

# Safety Data Sheet

# 4-Nitroquinoline- 1-oxide

Division of Safety  
National Institutes  
of Health



## WARNING!

THIS COMPOUND IS CARCINOGENIC AND MUTAGENIC. AVOID FORMATION AND BREATHING OF DUSTS.

LABORATORY OPERATIONS SHOULD BE CONDUCTED IN A FUME HOOD, GLOVE BOX, OR VENTILATED CABINET.

AVOID SKIN CONTACT: IF EXPOSED, WASH WITH SOAP AND WATER.

FOR EYE EXPOSURE, IRRIGATE IMMEDIATELY WITH LARGE AMOUNTS OF WATER. FOR INGESTION, DRINK PLENTY OF WATER OR MILK. INDUCE VOMITING. FOR INHALATION, REMOVE VICTIM PROMPTLY TO CLEAN AIR. ADMINISTER RESCUE BREATHING IF NECESSARY. REFER TO PHYSICIAN.

IN CASE OF LABORATORY SPILL, WEAR PROTECTIVE CLOTHING DURING CLEANUP. AVOID SKIN CONTACT OR BREATHING OF DUST. USE WATER TO DISSOLVE COMPOUND. WASH DOWN AREA WITH SOAP AND WATER. DISPOSE OF WASTE SOLUTIONS AND MATERIALS APPROPRIATELY.

### A. Background

4-Nitroquinoline-1-oxide (4-NQO) is a yellow crystalline solid. It is a potent carcinogen in animals and a mutagen in the Ames and other in vitro tests.

### B. Chemical and Physical Data

1. Chemical Abstract No.: 56-57-5

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2. Synonyms:

NQO

4-Nitroquinoline-N-oxide

4-NQO

Quinoline, 4-nitro-, 1-oxide (9CI)

3. Molecular

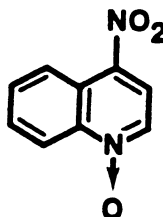
formula:

$C_9H_6O_3N_2$

weight:

190.17

structure:



4. Density: No data.

5. Absorption spectroscopy: Visible and UV (Okuno, 1972), IR (Costa et al., 1955), mass (Abramovitch and Smith, 1975), and fluorescence spectra (Yamane et al., 1972) have been reported.

6. Volatility: No data.

7. Solubility: Soluble in water, ethanol, acetone, and cyclohexane.

8. Description, appearance: Yellow needles or plates.

9. Boiling point: No data.

Melting point: 153-154°C.

10. Stability: No data.

11. Chemical reactivity: The most significant reactions are nucleophilic substitution of the nitro group by halogens and oxygen-, sulfur-, and nitrogen-containing groups; reduction of the nitro group (via 4-hydroxy-aminoquinoline-1-oxide) to 4-aminoquinoline-1-oxide; and deoxygenation of the N-oxide group.

12. Flash point: No data.

13. Autoignition temperature: No data.

14. Explosive limits in air: No data.

Fire, Explosion, and Reactivity Hazard Data

1. 4-NQO does not require special fire-fighting procedures or equipment and does not present unusual fire and explosion hazards.

2. No conditions contributing to instabilities, incompatibilities, or hazardous decomposition products have been reported.

3. 4-NQO has a low vapor pressure and does not require nonspark equipment. When handled in flammable solvents, the precautions required for such solvents apply.

### Operational Procedures

The NIH Guidelines for the Laboratory Use of Chemical Carcinogens describe operational practices to be followed when potentially carcinogenic chemicals are used in NIH laboratories. The Guidelines should be consulted to identify the proper use conditions required and specific controls to be implemented during normal and complex operations or manipulations involving 4-NQO.

1. Chemical inactivation: No validated method reported.
2. Decontamination: Turn off equipment that could be affected by 4-NQO or the materials used for cleanup. If more than 1 g has been spilled or if there is any uncertainty regarding the procedures to be followed for decontamination, call the NIH Fire Department (dial 116) for assistance. Wash surfaces with copious quantities of water. Glassware should be rinsed (in a hood) with ethanol, followed by soap and water. Animal cages should be washed with water.
3. Disposal: No waste streams containing 4-NQO shall be disposed of in sinks or general refuse. Surplus 4-NQO or chemical waste streams contaminated with 4-NQO shall be handled as hazardous chemical waste and disposed of in accordance with the NIH chemical waste disposal system. Nonchemical waste (e.g., animal carcasses and bedding) containing 4-NQO shall be handled and packaged for incineration in accordance with the NIH medical-pathological waste disposal system. Potentially infectious waste (e.g., tissue cultures) containing 4-NQO shall be disinfected by heat using a standard autoclave treatment and packaged for incineration, as above. Burnable waste (e.g., absorbent bench top liners) minimally contaminated with 4-NQO shall be handled as potentially infectious waste and packaged for incineration, as above. Absorbent materials (e.g., associated with spill cleanup) grossly contaminated shall be handled in accordance with the chemical waste disposal system. Radioactive waste containing 4-NQO shall be handled in accordance with the NIH radioactive waste disposal system.
4. Storage: Store in closed containers, preferably under refrigeration.

### Monitoring and Measurement Procedures Including Direct Field Measurements and Sampling for Subsequent Laboratory Analysis

1. Sampling: Since 4-NQO is used only under laboratory conditions, methods for field sampling and measurement have not been developed.

2. Separation and analysis: Analysis may be based on UV and visible spectrometry (Okuno et al., 1972). Determination in biological material, by means of benzene extraction and fluorescence measurement, with a detectability range of 1-25 ppm, has been reported (Yamane et al., 1972).

### Biological Effects (Animal and Human)

1. Absorption and distribution: No data; nearly all toxic (carcinogenic) effects occur at or near the site of application. However, the reported appearance of lung tumors following intraperitoneal injection of 4-NQO may imply some absorption and distribution.
2. Metabolism and excretion: 4-NQO is reduced in vivo (subcutaneous injection) and in vitro (liver homogenates) through 4-hydroxyamino quinoline-1-oxide to 4-aminoquinoline-1-oxide and is metabolized to 4-hydroxyquinoline-1-oxide (Endo et al., 1971). Indirect evidence indicates that the hydroxylamino derivative may be the molecular species responsible for the carcinogenicity of 4-NQO. There are no data on excretion of 4-NQO or any of its metabolites.
3. Toxic effects: No data on acute toxicity. Subcutaneous 4-NQO causes immunosuppression in mice, apparently through inhibition of synthesis of complement components. Intraperitoneal 4-NQO produces severe necrosis in rat pancreas, salivary glands, and lungs.
4. Carcinogenic effects: These have been reviewed (Nagao and Sugimura, 1976). Topical application produces local epithelial carcinomas (skin, palate, kidney, stomach). Tumors are produced in the offspring of mice by transfer through the placenta and milk.
5. Mutagenic and teratogenic effects: 4-NQO is active in the Ames test and is mutagenic in many lower species, though not in mice. There is no evidence for teratogenicity.

### Emergency Treatment

1. Skin and eye exposure: For skin exposure, remove contaminated clothing and wash skin with soap and water. For eye exposure, irrigate immediately with copious quantities of running water for at least 15 minutes.
2. Ingestion: Drink plenty of water or milk. Induce vomiting.
3. Inhalation: Remove victim promptly to clean air. Administer rescue breathing if necessary.
4. Refer to physician. Consider treatment for pulmonary irritation.

## References

- Abramovitch, R.A., and E.M. Smith. 1975. 4-Nitrosoquinoline-1-oxide. *J Heterocyc Chem* 12:969-972.
- Costa, G., P. Blasina, and G. Sartori. 1955. Infrared spectra of substituted quinoline derivatives and their N-oxides. *Univ Stud Trieste Fac Sci 1st Chim* (9):11.
- Endo, H., T. Ono, and T. Sugimura, eds. 1971. *Recent Results in Cancer Research: Chemistry and Biological Actions of 4-Nitroquinoline-1-Oxide*. Springer-Verlag, New York.
- Nagao, M., and T. Sugimura. 1976. Molecular biology of the carcinogen, 4-nitroquinoline-1-oxide. *Adv Cancer Res* 23:131-169.
- Okuno, T., M. Goto, H. Matsumoto, and A. Takadate. 1972. Electronic properties of N-heteroaromatics. XLVII. Absorption spectra and electronic structures of some quinoline-1-oxides of biological interest. *Chem Pharm Bull* 20:2551-2560.
- Yamane, Y., M. Ohtawa, and M. Iigo. 1972. Determination of 4-nitroquinoline-1-oxide and its metabolites in biological materials. *Yakugaku Zasshi* 92:631-634.